S205 The molecular world

S343 Inorganic chemistry

S344 Organic chemistry: a synthesis approach

The Open University

Making molecular models with the Orbit model kit

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5.1

1 Introduction

Included in your first S205 course mailing you will find an Orbit (molecular) model kit. The model kit will be useful throughout your study of each of the courses S205, S343 and S344 and the associated residential schools, SXR205, SXR343 and SXR344. With the kit you will be able to construct models of most of the structures discussed in each course. It would therefore be useful to have the kit to hand during all your study periods.

2 Notes on the model kit

The model kit contains two types of component: atom centres, which are small plastic spheres or cylinders with prongs (arms), and coloured plastic straws (mainly grey) to represent bonds. Each of the eight types of atom centre can represent a number of different atoms, and they are colour-coded, as indicated in Table 1.

2.1 Bonds

The grey straws are for constructing standard covalent bonds between atoms. They simply push onto the arms on the atom centres to form bonds. If this is difficult when the straws are new, moisten the ends of the arms.

A covalent bond between two atoms is represented by a grey straw with two appropriately coloured atom centres, one at each end. Molecular models are constructed by joining the appropriate centres together in the order indicated by their structural formula; examples of how to construct particular molecular models are given in Table 2. When making molecular models, always bear in mind that a properly constructed molecule should have no 'free' prongs.

To construct multiple bonds, use the white bonding pegs. Double bonds, for instance, can be made by inserting two such pegs into the two atom centres at either end of the bond, and connecting them by a straw.

Straws of four different lengths are provided. The most convenient scale for bond lengths is 2 cm ≡ 100 pm (10^{-10} m or 1 Å). Using this scale, the pre-cut straws that are 3 cm long are used for C—C single bonds (*c*. 154 pm), bonds between second-row elements, or between hydrogen and third-row elements. Those that are 2.5 cm long correspond to C=O double bonds (*c*. 125 pm), or bonds between hydrogen and the second-row elements. Those that are 2 cm long correspond to C—H bonds (*c*. 107 pm). The 5 cm straws should be used for longer bonds such as C—Cl, C—Br, etc. However, you will probably be using the 5 cm straws most of the time, especially when you only need to show the stereochemistry of molecules.

Provided the ratio of bond lengths within your model is roughly accurate, any combination of the lengths provided can be used.

The flexible white tubes are specifically for constructing strained systems or bonds of a non-standard shape; for example, the 'banana' bonds of cyclopropane rings, and bidentate ligands.

Table 1 Contents of the molecular model kit.

Atom centre type	Colour	Element
one-coordinate 	white	hydrogen atom, —H
	blue	nitrile nitrogen, ≡N
	red	carbonyl oxygen, =O
	yellow	double-bonded sulfur, =S
	light green	fluorine atom, —F
	green	chlorine atom, —Cl
	dark green	bromine atom, —Br
	very dark green	iodine atom, —I
two-coordinate (linear)	white	hydrogen bond, —H···
	black	alkyne carbon, ≡C—
	black	alkene carbon =C=
	blue	half-azo nitrogen, —N=
two-coordinate (100°) 	yellow	saturated divalent sulfur, —S—
two-coordinate (120°) 	red	saturated oxygen atom, —O—
trigonal (120°) 	black	planar carbon (alkene or aromatic), $=C\begin{matrix}/\\\backslash\end{matrix}$
	blue	planar nitrogen, $=N\begin{matrix}/\end{matrix}$
	red	planar oxygen, =O

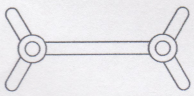
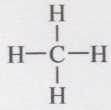
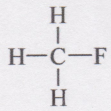
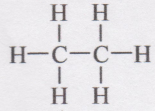
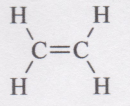
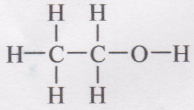
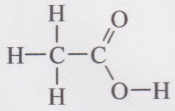
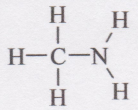
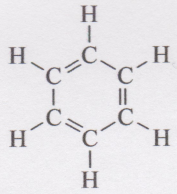
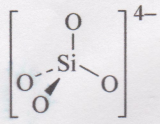
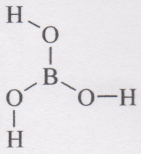
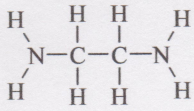
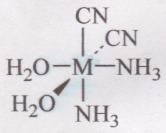
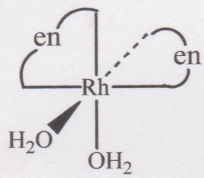
Atom centre type	Colour	Element
tetrahedral 	black	saturated carbon
	blue	positively charged nitrogen, or R_3N, showing non-bonded electron pair
	red	four-coordinate oxygen, R_2O, showing two non-bonded electron pairs
	yellow	sulfur (e.g. RSO_3H or RSH, showing non-bonded electron pair)
	purple	four-coordinate phosphorus (e.g. $R_3P{=}O$)
	silver	tetrahedral metal atom; also use for three-coordinate and lone-pair, or two-coordinate and two lone-pairs
trigonal bipyramidal	purple	five-coordinate nitrogen, five-coordinate oxygen, five-coordinate phosphorus; also use for four-coordinate and lone-pair, or three-coordinate and two lone-pairs
octahedral 	black	octahedral
	red	octahedral
	yellow	octahedral sulfur
	green	octahedral halogen
	silver	octahedral metal: also use for five-coordinate plus lone-pair, and for four-coordinate and two lone-pairs
orbital shape 	black and white	orbital lobes for p orbitals (π-bonding and for lone-pairs)
planar double atom 	black	for alkenes

Table 2 How to construct various molecular models with the Orbit kit.

Molecule	Molecular formula	Structural formula	Kit parts	Advice
hydrogen	H_2	H—H	2 H centres 1 grey straw	Attach an H centre to either end of the straw.
chlorine	Cl_2	Cl—Cl	2 Cl centres 1 grey straw	Similar to above.
oxygen	O_2	O=O	2 O centres 2 white tubes	Similar to above, but use a flexible white tube. Join the remaining free prongs on each O centre with the second flexible white tube.
nitrogen	N_2	N≡N	2 N centres 3 white tubes	Similar to O_2 above, but use the three flexible tubes to join the two N centres together.
water	H_2O		2 H centres 1 O centre *or* tetrahedral centre 2 grey straws	Use one grey straw to join one H centre to a prong on the O centre. Use another grey straw to join the second H centre to the second prong on the O centre. The model should be V-shaped. If using a tetrahedral centre, attach two lone-pairs.
methane	CH_4		4 H centres 1 C centre 4 grey straws	Attach a grey straw to each of the four prongs on the C centre. Attach an H centre to the free end of each straw.
fluoromethane	CH_3F		3 H centres 1 F centre 1 C centre 4 grey straws	As for methane, but replace one H centre with an F centre.
ethane	C_2H_6		6 H centres 2 C centres 7 grey straws	Join the C centres together with a grey straw. Attach grey straws to the remaining six prongs. Attach H centres to the free ends of the six grey straws.
ethene	C_2H_4		4 H centres 2 C centres 4 grey straws 2 white tubes *or* use the planar double atom centre	Join the C centres together with two flexible white tubes. Attach grey straws to the remaining four prongs (two on each C centre). Attach H centres to the free ends of the four grey straws.

Molecule	Molecular formula	Structural formula	Kit parts	Advice
ethanol	CH_3CH_2OH		6 H centres 2 C centres 1 O centre 8 grey straws	As for ethane, but replace one H centre with an O centre. Attach a grey straw with an H centre to the free prong on the O centre.
ethanoic acid	CH_3COOH		4 H centres 2 C centres 2 O centres 6 grey straws 2 white tubes	As for ethanol, but replace the two H centres connected to the C centre attached to the O—H group with a single O centre. This new C=O double bond should be constructed using two flexible white tubes.
methylamine	CH_3NH_2		5 H centres 1 C centre 1 N centre 6 grey straws	As for methane, but replace one H centre with an N centre. Attach two grey straws each with an H centre to the two free prongs on the N.
benzene	C_6H_6		6 H centres 6 C centres 9 grey straws 6 white tubes *or* use 6 trigonal bi-pyramidal centres and 6 p orbitals *or* 3 planar double-atom centres	Join the six C centres together in a hexagonal ring, using grey straws (three) and flexible white tubes (three) alternately. Make three alternate double bonds by further joining each of the C centre 'white-bonded' pairs with another white tube. This should leave each C centre with a single free prong, to which you should attach a grey straw with an H centre. Using the trigonal bipyramids enables the p-orbitals to be attached.
difluoro selenium oxide	F_2SeO		2 F centres 1 O centre (4 prong) 1 Se centre (blue) 3 grey straws	Attach the three grey straws to the tetrahedral Se centre, and add the two F and O centres to the ends of each straw. Attach an orbital shape to the remaining prong to represent a non-bonded pair of electrons on selenium. Note that the Se is joined to O by a double bond, in contrast to the two Se—F single bonds.

Molecule	Molecular formula	Structural formula	Kit parts	Advice
silicate ion	SiO_4^{4-}		4 O centres (4 prong) 1 Si centre (silver) 4 grey straws	Attach the four grey straws to the tetrahedral Si centre, and add the four tetrahedral O centres to the ends of each straw. *Note* As this is a complex ion, a tetrahedral O centre is used, two of the prongs of which represent normal non-bonded electron pairs on the oxygen while the remaining prong 'accommodates' the four electrons that give the complex ion its charge of 4–.
boric acid	H_3BO_3		1 B centre (blue) 3 O centres 3 H centres 6 grey straws	Attach three of the grey straws to the trigonal B centre. Attach a grey straw to each of the O centres, and add the three H centres to the ends of each straw. Add the three O—H groups to the grey straws connected to the B centre.
ethylene-diamine	$H_2N(CH_2)_2NH_2$		2 C centres 2 N centres (4 prong) 8 H centres 11 grey straws	Join the two tetrahedral C centres using a grey straw. Attach six grey straws to the remaining prongs. Attach two grey straws to each tetrahedral N centre (one of the remaining prongs represents the non-bonded electron pair on each nitrogen), and add an H centre to each of the grey straws on each N centre. Attach each NH_2 to each one of the C centres, and add the four remaining H centres to complete the methylene group for each C centre.

Molecule	Molecular formula	Structural formula	Kit parts	Advice
diammine-diaquodicyano M(II)			2 C centres (2 prong) 2 N centres (4 prong) 2 N centres (2 prong) 10 H centres 2 O centres (4 prong) 1 M centre (6 prong, silver) 16 grey straws (standard) 2 grey straws (short)	Attach each short grey straw to each linear C centre, and add a two-prong N centre to each straw; this is a simplified form of the CN ligand with a non-bonded pair of electrons on the nitrogen represented by the unconnected prong. Attach four grey straws to each tetrahedral N centre, and add three H centres to each to produce two NH_3 ligands. Attach two grey straws to each tetrahedral O centre, and add two H centres to each to produce two H_2O ligands (the additional prong on each O centre represents a non-bonding electron pair). Attach the remaining six grey straws to the octahedral M centre, and complete the model by attaching all the ligands prepared above.
diaquobis-(1,2-di-aminoethane)-rhodium(0)			4 N centres (4 prong) 4 C centres 2 O centres (4 prong) 20 H centres 1 Rh centre (black) 32 grey straws *or* 2 flexible white straws	Construct two models of the ethylenediamine (en) ligand, using a similar procedure to that employed for ethylenediamine above. Construct two H_2O ligands. Attach six grey straws to the octahedral Rh centre. Complete the model by attaching the four ligands to the Rh centre. Alternatively use a flexible white straw to represent en.